LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.237	489	493	503	rVB	45067	52293	1.48%	0.256%
2	5.625	555	559	571	rBV	1132649	989828	28.09%	4.843%
3	6.613	724	727	731	rBV	665233	609313	17.29%	2.981%
4	6.766	749	753	757	rBV	2044575	1829526	51.92%	8.952%
5	7.001	789	793	796	rBV	743242	658623	18.69%	3.223%
6	7.154	815	819	823	rBV	2759598	2661392	75.53%	13.023%
7	7.566	883	889	892	rBV	2103669	2108496	59.84%	10.317%
8	8.284	1007	1011	1014	rBV	842088	719284	20.41%	3.520%
9	9.354	1189	1193	1197	rBV	3799832	3523552	100.00%	17.241%
10	9.748	1256	1260	1271	rVB	82657	83304	2.36%	0.408%
11	10.042	1307	1310	1317	rVB2	800713	688855	19.55%	3.371%
12	10.701	1419	1422	1427	rBV	48058	40228	1.14%	0.197%
13	10.836	1441	1445	1457	rBV	1174109	1098551	31.18%	5.375%
14	11.536	1560	1564	1572	rBV	697587	616103	17.49%	3.015%
15	13.124	1829	1834	1837	rBV	3232711	2744767	77.90%	13.431%
16	13.671	1924	1927	1930	rBV	54406	48186	1.37%	0.236%
17	14.001	1980	1983	1986	rBV	67774	53843	1.53%	0.263%
18	14.060	1986	1993	2005	rBV5	42761	148091	4.20%	0.725%
19	14.189	2011	2015	2021	rBV	758466	713649	20.25%	3.492%
20	14.319	2033	2037	2040	rBV	91098	79108	2.25%	0.387%
21	14.624	2086	2089	2093	rBV	103433	99765	2.83%	0.488%
22	14.948	2141	2144	2151	rVB	92363	94909	2.69%	0.464%
23	15.030	2155	2158	2162	rVB	57555	61985	1.76%	0.303%
24	15.313	2202	2206	2212	rVB	78448	89729	2.55%	0.439%
25	15.748	2271	2280	2288	rBV	326076	553882	15.72%	2.710%
26	16.195	2351	2356	2361	rVB2	42635	69228	1.96%	0.339%

Sum of corrected areas: 20436490

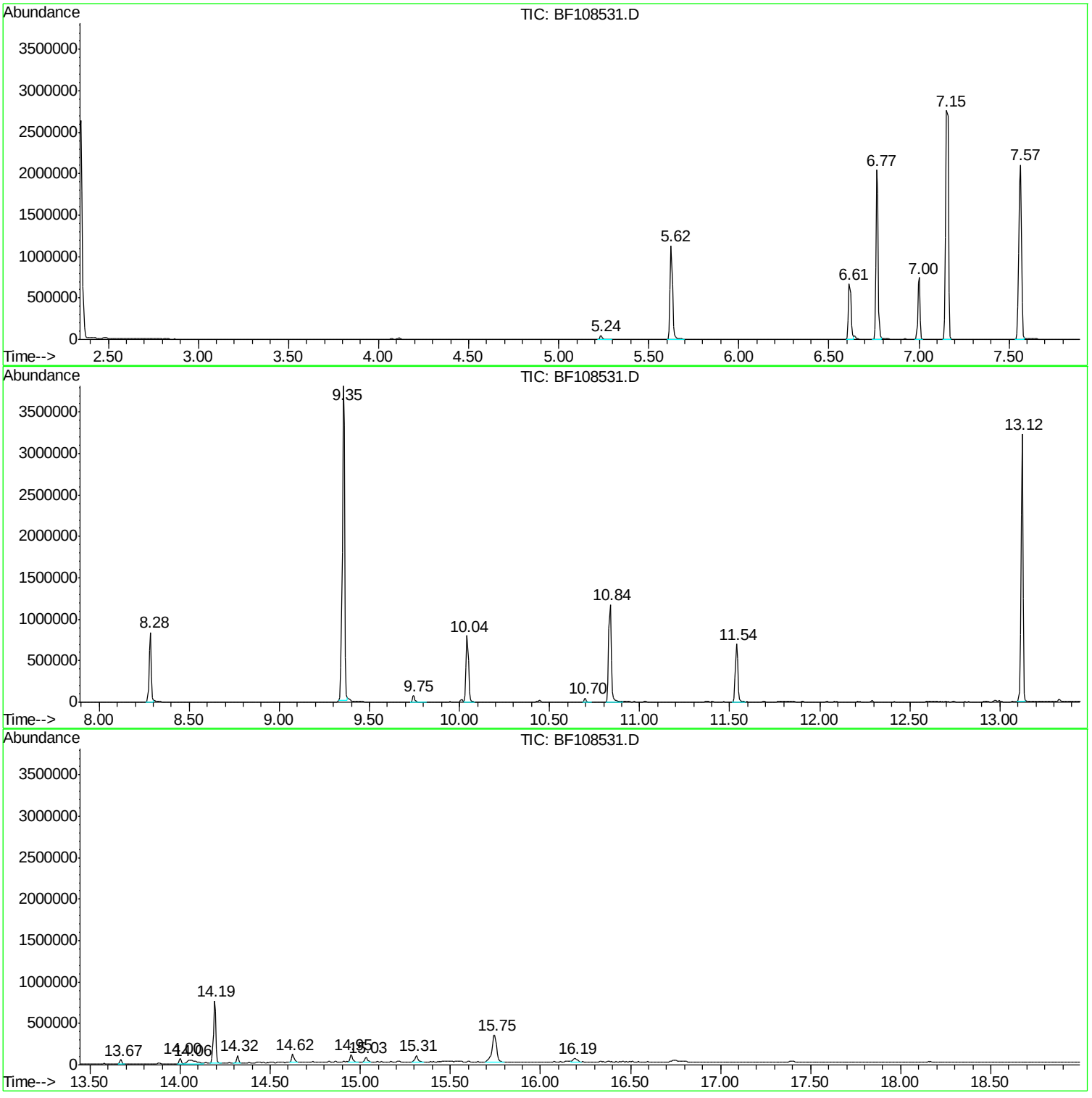
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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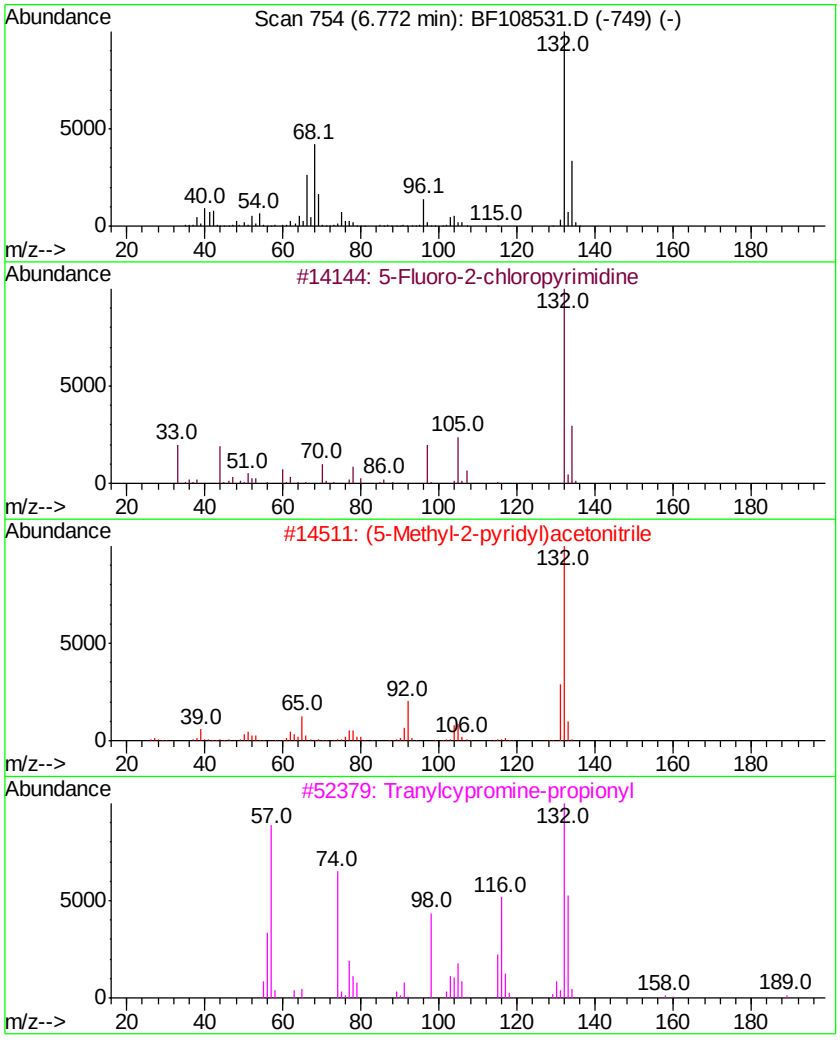
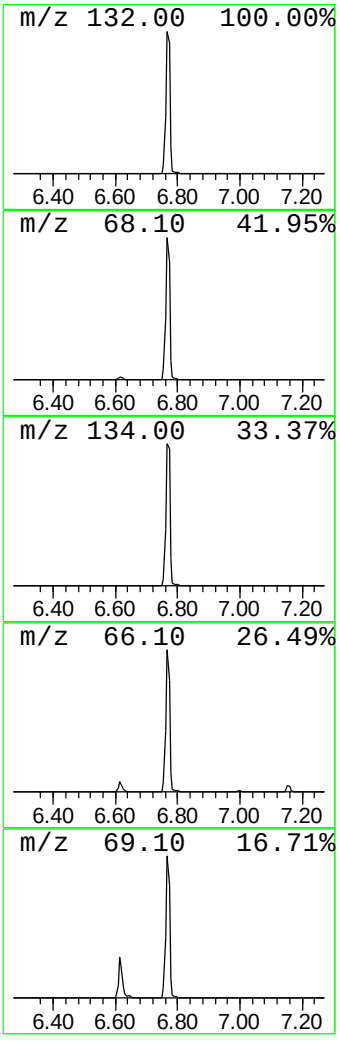
Peak Number 1 unknown6.77 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	55.56 ng	1829530	1,4-Dichlorobenzene-d4	7.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
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Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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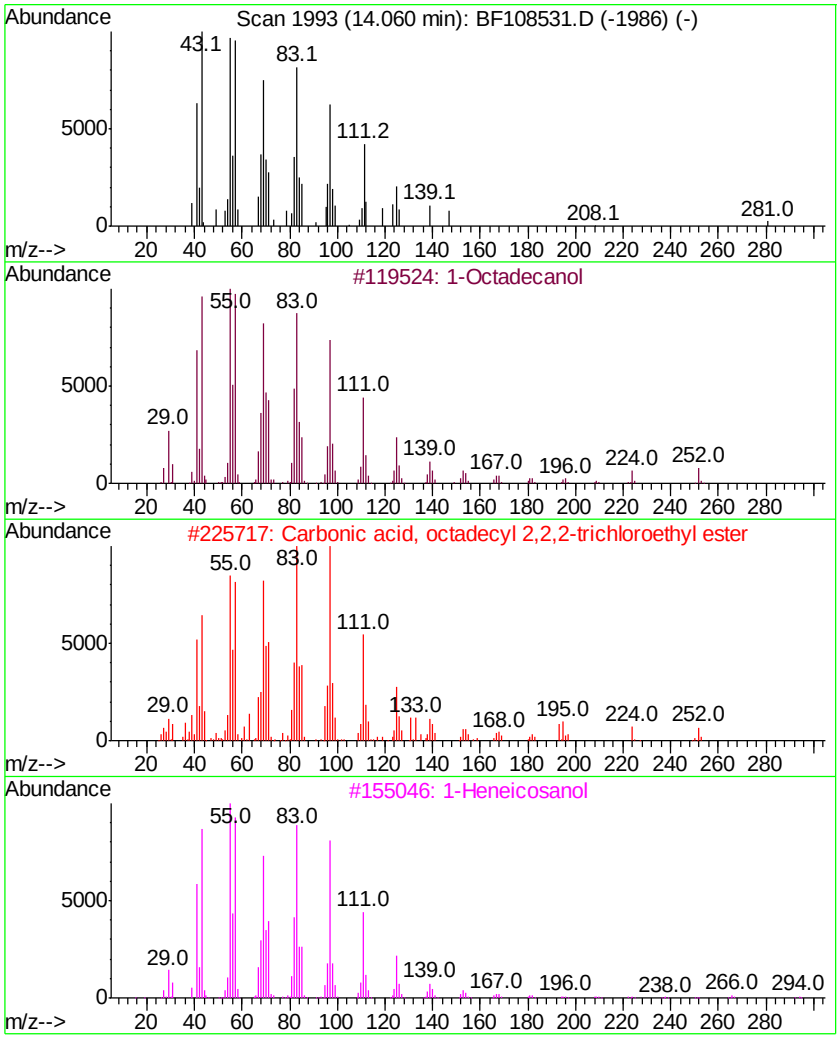
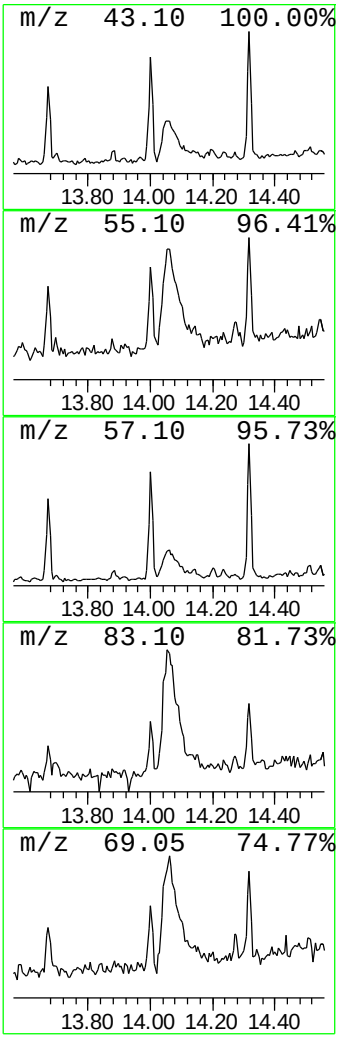
Peak Number 3 1-Octadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	4.15 ng	148091	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	94
2	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	93
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Behenic alcohol	326	C22H46O	000661-19-8	91
5	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	91





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Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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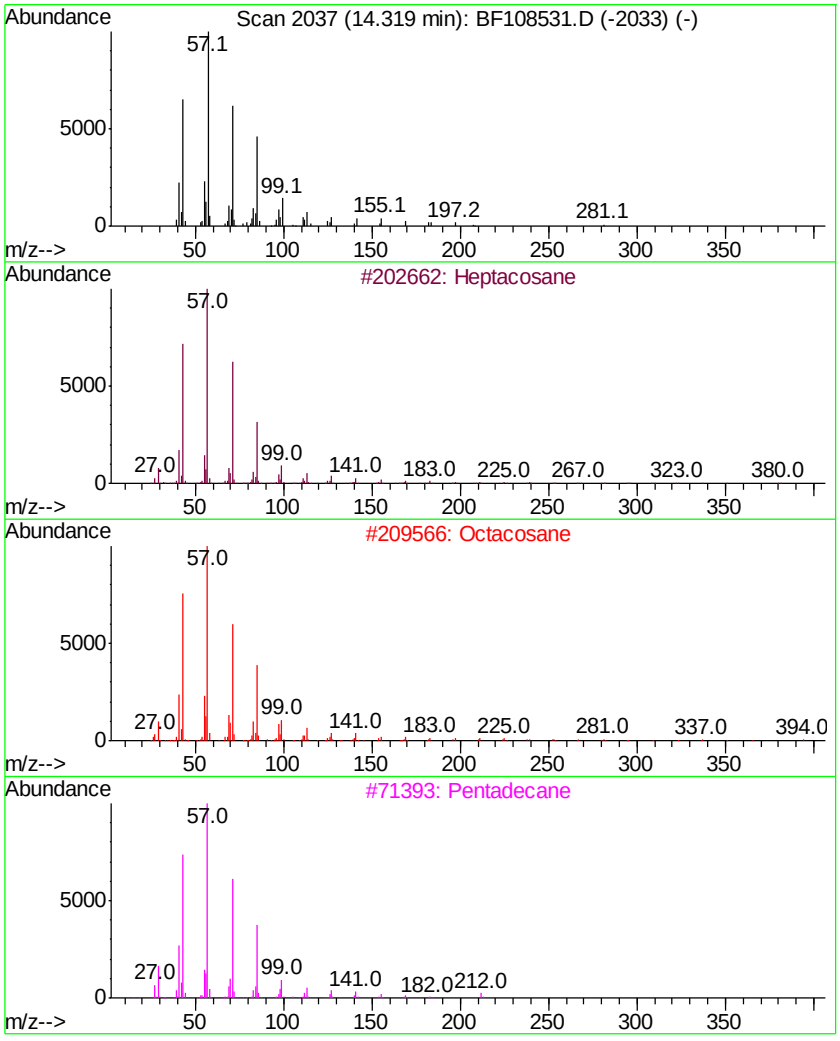
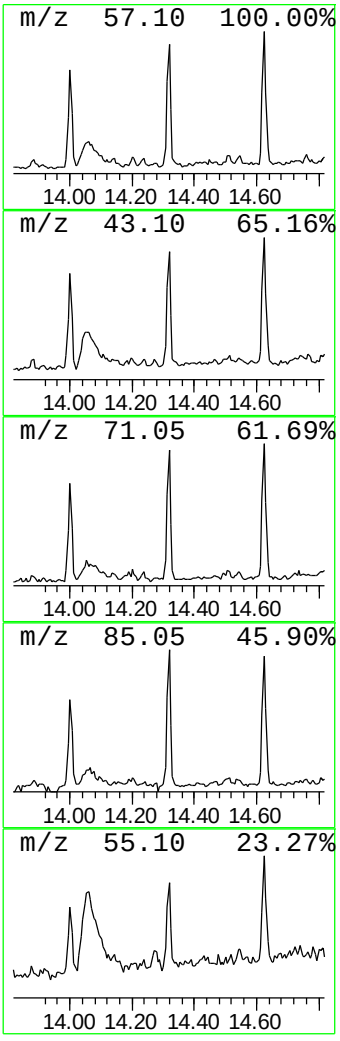
Peak Number 4 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.32	2.22 ng	79108	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentadecane	212	C15H32	000629-62-9	91
4	Octadecane	254	C18H38	000593-45-3	91
5	Hexadecane	226	C16H34	000544-76-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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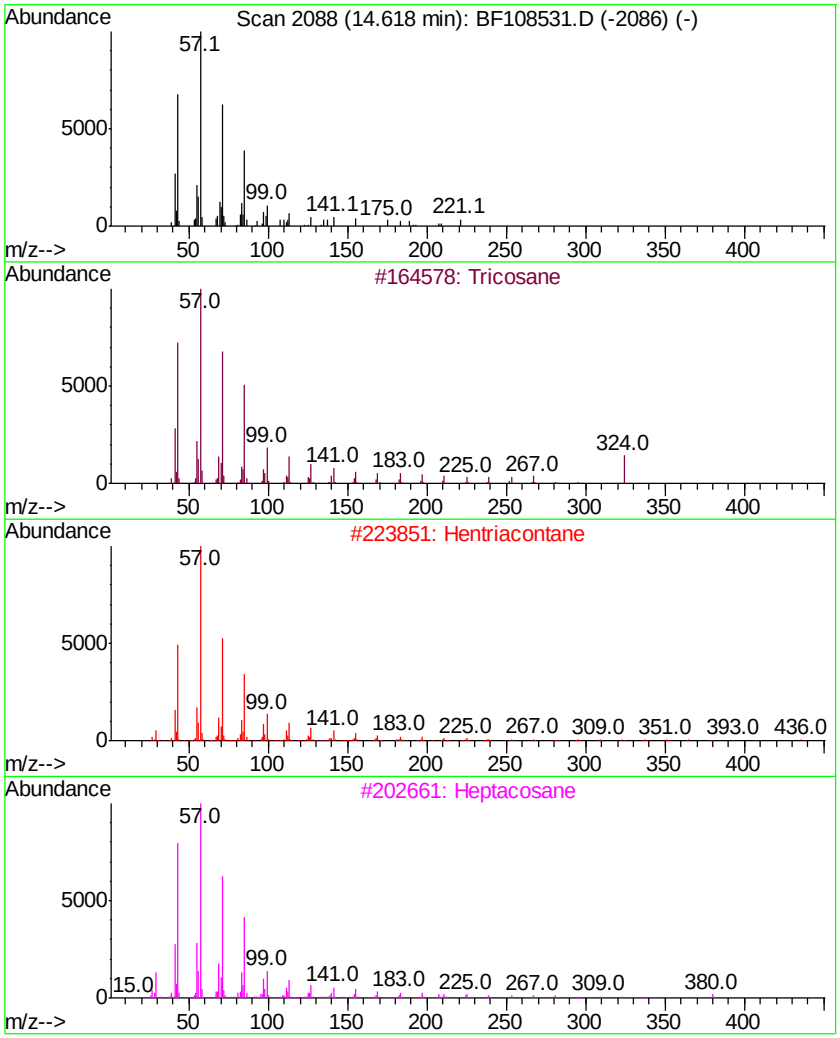
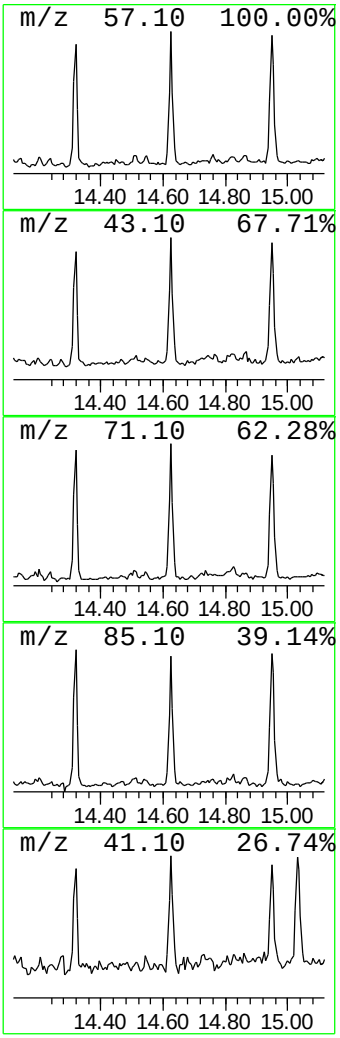
Peak Number 5 Tricosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.80 ng	99765	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane	324	C23H48	000638-67-5	93
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

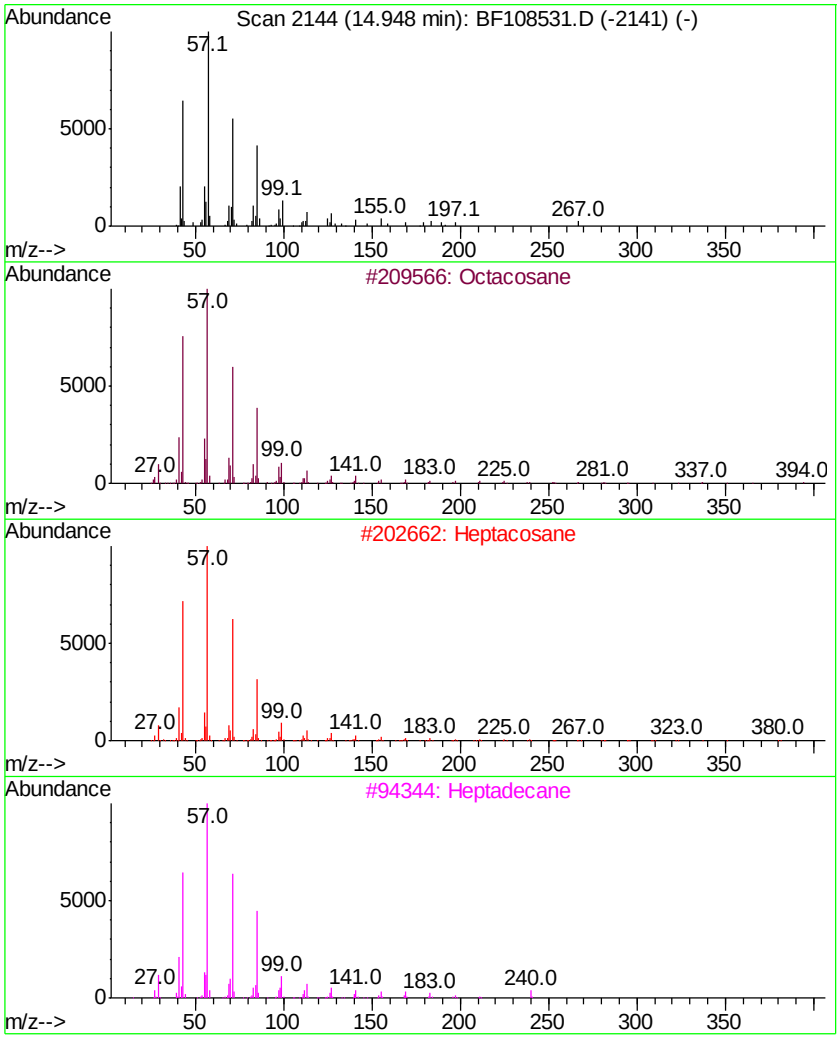
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

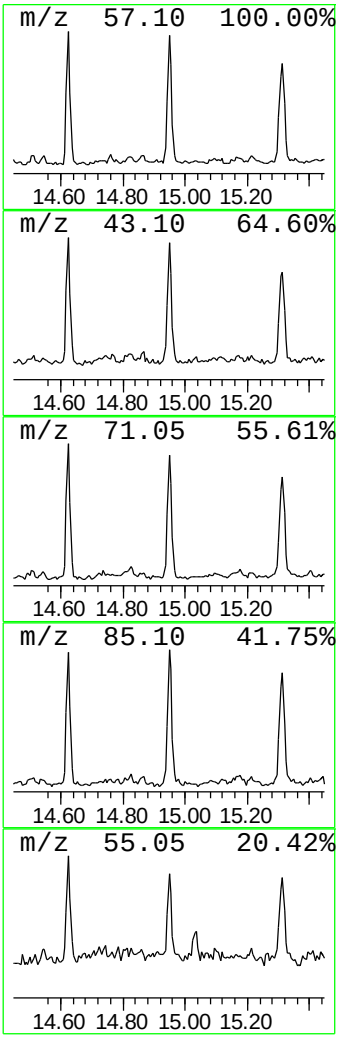
****

Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.66 ng	94909	Chrysene-d12	14.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetracosane	338	C24H50	000646-31-1	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

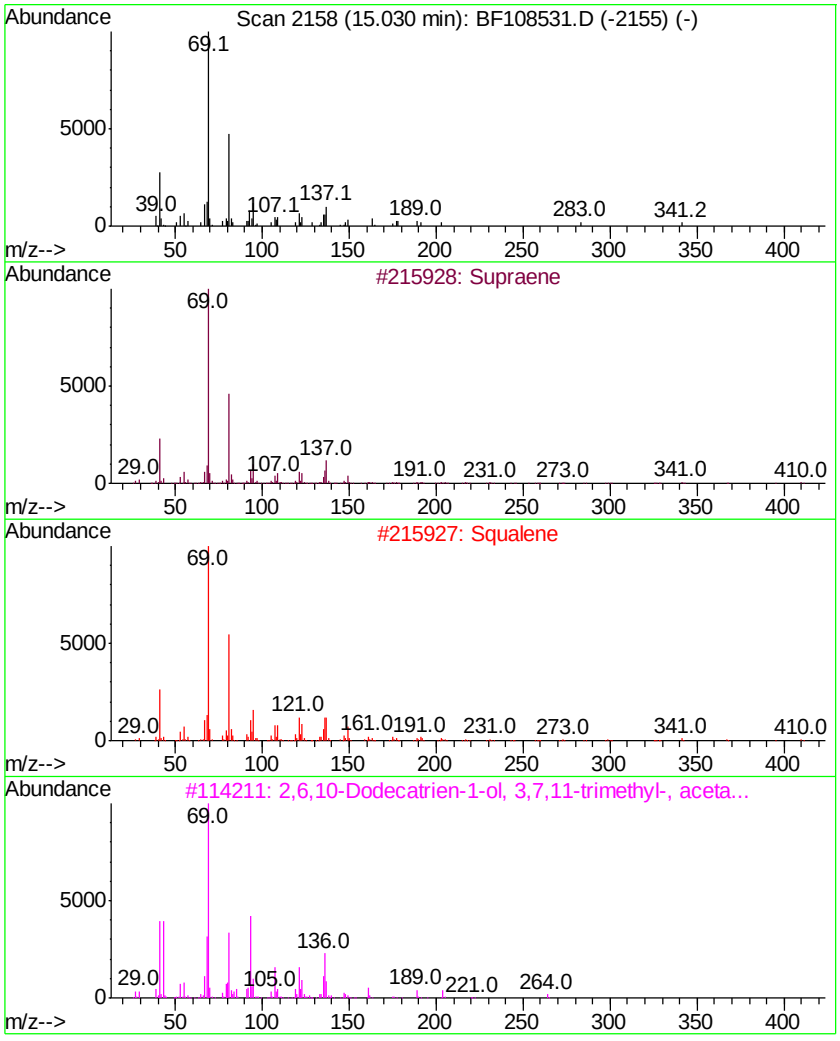
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

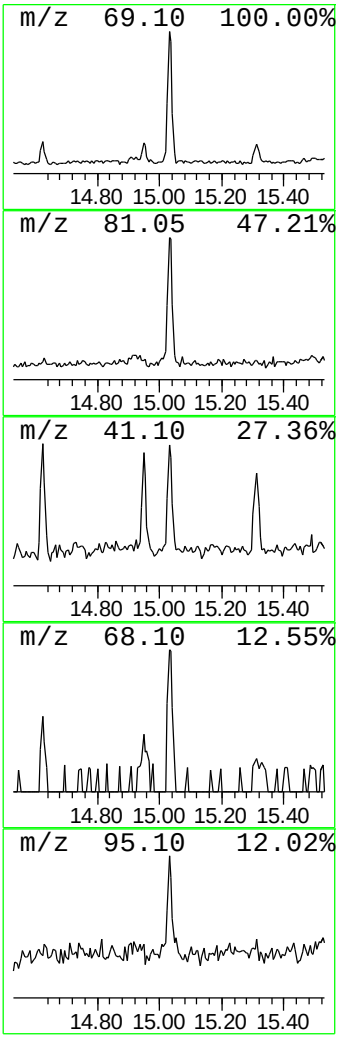
****

Peak Number 7 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.03	2.24 ng	61985	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	83
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	50
4	Crotonoyl bromide	148	C4H5BrO	055600-70-9	50
5	1,5-Heptadiene, 2,6-dimethyl-	124	C9H16	006709-39-3	40





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
Operator : JU/SJ
Sample : J4659-04
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

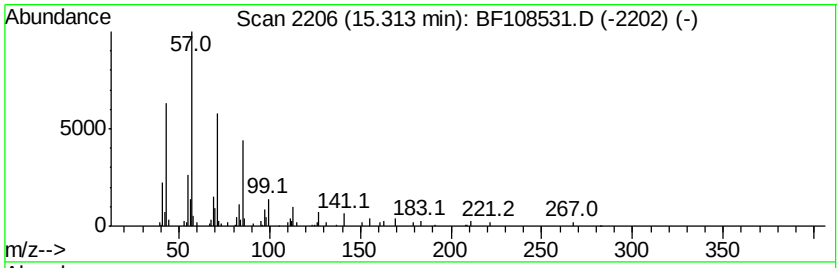
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

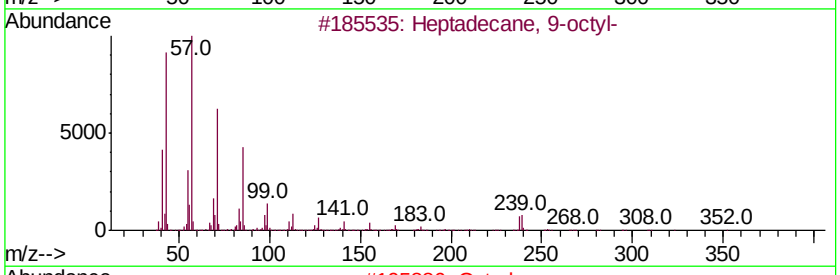
****

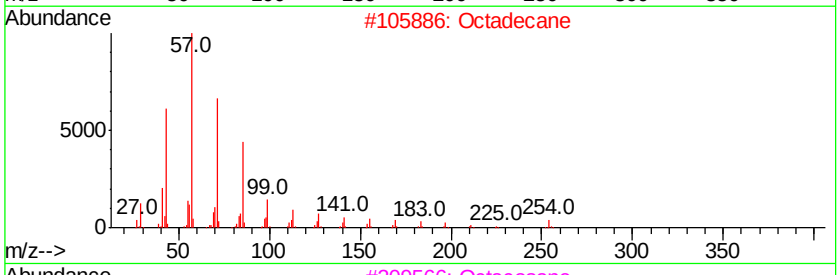
Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 4

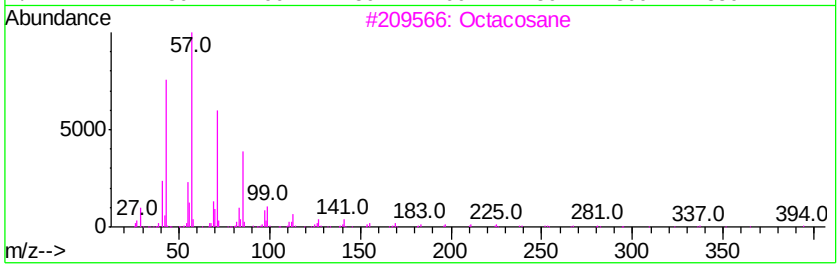
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	3.24 ng	89729	Perylene-d12	15.75

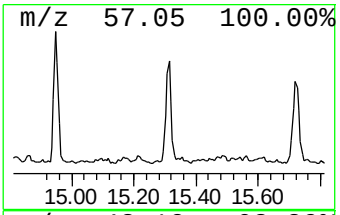
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Octadecane	254	C18H38	000593-45-3	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Docosane	310	C22H46	000629-97-0	90
5	Heptadecane	240	C17H36	000629-78-7	90

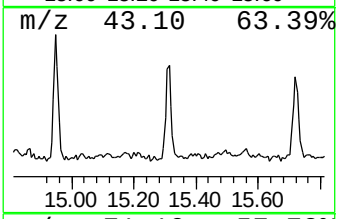


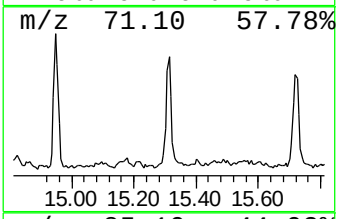


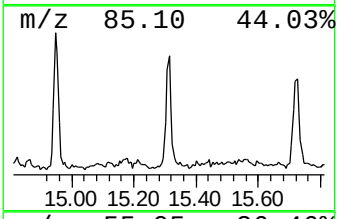


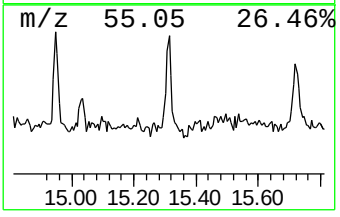












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Acq On : 28 Aug 2018 1:28
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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 082218-TIPC-F-U-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

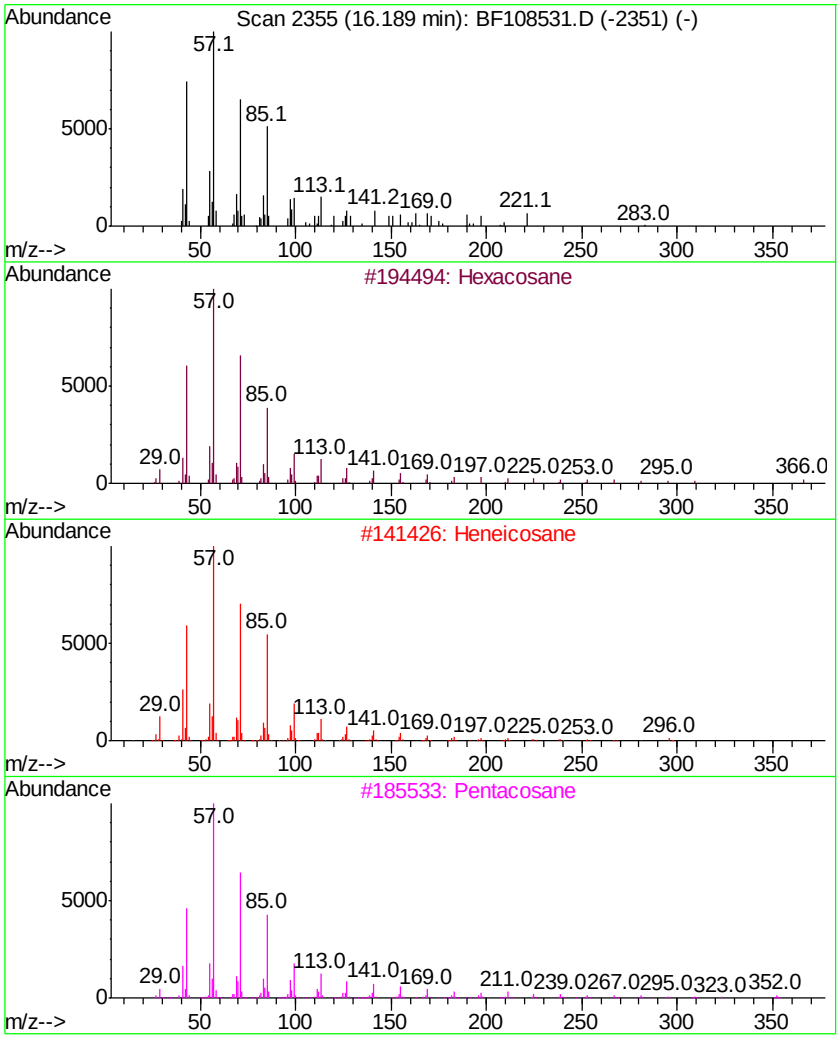
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

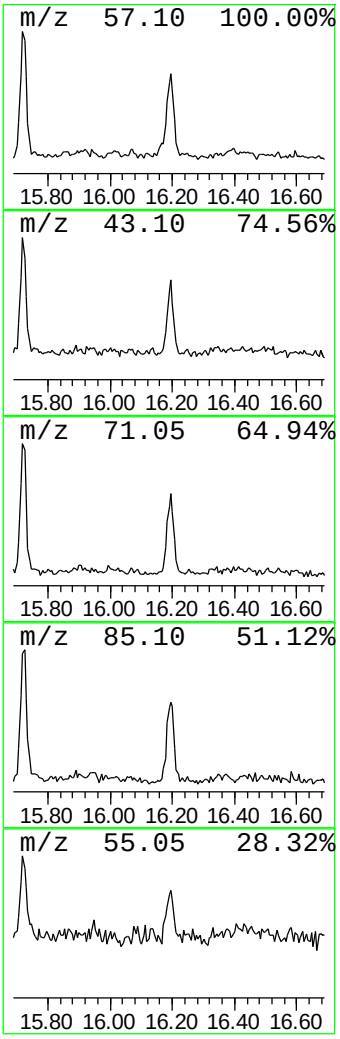
****

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.50 ng	69228	Perylene-d12	15.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Pentacosane	352	C25H52	000629-99-2	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Octacosane	394	C28H58	000630-02-4	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082718\
Data File : BF108531.D
Acq On : 28 Aug 2018 1:28
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Instrument : BNA_F
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.77	6.77	55.6	ng	1829530	1	7.00	658623	20.0
1-Octadecanol	14.06	4.2	ng	148091	5	14.19	713649	20.0
Heptacosane	14.32	2.2	ng	79108	5	14.19	713649	20.0
Tricosane	14.62	2.8	ng	99765	5	14.19	713649	20.0
Octacosane	14.95	2.7	ng	94909	5	14.19	713649	20.0
Supraene	15.03	2.2	ng	61985	6	15.75	553882	20.0
Heptadecane, 9-oc...	15.31	3.2	ng	89729	6	15.75	553882	20.0
Hexacosane	16.19	2.5	ng	69228	6	15.75	553882	20.0